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A finite element recovery approach to Green's function approximations with applications to electrostatic potential computation[☆]

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ABSTRACT

In this paper, a finite element recovery approach is proposed to improve the accuracy of finite element approximations for Green's functions in three dimensions. This recovery approach is based on some simple postprocessing. It is proved by both theory and numerics that the recovery approach is very efficient. In particular, the approach is successfully applied to some electrostatic potential computations.

1. Introduction

Electrostatics plays a fundamental role in virtually all processes involving biomolecules in solution. One of the main approaches to treat electrostatic effects in solution is the so-called Poisson–Boltzmann equation (PBE), which is a nonlinear singular elliptic partial differential equation. We refer to [11,12,15,17,22,26–28] and references cited therein for the state of art in studying electrostatics based on the PBE.

Since the analytic solution of the PBE only exists in very few cases for simple shape molecules, numerical solutions of the PBE become natural. In solving the PBE, however, there exist many difficulties that need to be overcome, including the coefficient discontinuity, the exponential nonlinearity, the three spatial dimensions and a number of point singularities. It is shown that among the difficulties, the point singularity is the most difficult one. Consequently, the following linearized PBE is significant in electrostatic potential computations (see, e.g., [12,14,15,19,25,31]):

$$\begin{cases} -\nabla\left(\epsilon(x)\nabla\phi(x)\right)+\bar{\kappa}^2(x)\phi(x)=4\pi e_c\displaystyle\sum_{i=1}^{N_m} z_i\delta_{x_i}(x) \quad \text{in } \mathbb{R}^3, \\ \phi(\infty)=0. \end{cases} \tag{1.1}$$

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Here ϕ is the electrostatic potential, the permittivity ϵ takes different values of dielectric constants in the different regions (molecular region and solution region) of the model, the modified Debye–Hückel parameter $\bar{\kappa}$ takes the value $\sqrt{\epsilon_w}\kappa$ in the solution region and zero in the molecular region (where ϵ_w is the dielectric constant in the solution region and κ is the usual Debye–Hückel parameter), the constant e_c is the charge of an electron and z_i is the chemical valence of the charge located at x_i ($i = 1, \ldots, N_m$) in the molecule. For the past two decades, various numerical methods such as finite element methods (see, e.g., [3–5,9,10,16]), finite difference methods (see, e.g., [15,18,19]) and boundary element methods (see, e.g., [23,32]) have been proposed for both the original and the linearized PBEs. Among such approaches, the finite element method is considered to be very promising in that irregular shapes can be fitted more easily. Moreover, the finite element method allows fine meshes to be put where they are needed, such as at interfaces, and coarser meshes to be put far from the molecule, where spatial changes in electrostatic potential are small.

It is noted that the solution of (1.1) can be viewed as a sum of Green's functions ϕ_i ($i = 1, \ldots, N_m$) satisfying

$$\begin{cases} -\nabla\left(\epsilon(x)\nabla\phi_i(x)\right) + \bar{\kappa}^2(x)\phi_i(x) = 4\pi e_c z_i \delta_{x_i}(x) \quad \text{in } \mathbb{R}^3, \\ \phi_i(\infty) = 0. \end{cases} \tag{1.2}$$

However, the standard finite element solution of (1.2) fails to give a good approximation to Green's function ϕ_i in the vicinity of the singular point x_i. To construct highly accurate approximations for Green's function, in this paper, a recovery approach based on some simple postprocessing is proposed. Let us give a somewhat more detailed but informal description of the idea and result. For simplicity, consider a generic Green's function G_z associated with the singular point z that satisfies

$$\begin{cases} -\mathrm{div}(\alpha(x)\nabla G_z(x)) + \beta(x)G_z(x) = \delta_z(x) \quad \text{in } \Omega, \\ G_z = 0 \quad \text{on } \partial\Omega. \end{cases} \tag{1.3}$$

Then we are able to construct the so-called recovered approximation γ_h, which is obtained from the discrete Green's function G_z^h and has the following error estimate (see Theorem 3.1):

$$|G_z(x) - \gamma_h(x)| \le Ch\left(\left|\ln\frac{h}{d}\right|^2 + \left|\ln\frac{|x-z|}{d}\right|\right) \quad \text{if } 0 < |x-z| \le Ch \tag{1.4}$$

for a class of coefficients α and β, where C and d are some constants that are independent of h. While for the standard discrete Green's function G_z^h, we have only [24]:

$$|G_z(x) - G_z^h(x)| \le C\frac{1}{|x-z|} \quad \text{if } 0 < |x-z| \le Ch, \tag{1.5}$$

which obviously means that the constructed approximation γ_h is much better than G_z^h, as the approximation to G_z in the vicinity of singular point z. For an application, we successfully apply the above recovery approach to electrostatic potential computations (see Section 4). These numerical experiments demonstrate the efficiency of the approach and support our theory.

It should be mentioned that the recovery idea may be dated back to Peaceman [20,21], in which the well-known Peaceman technique in the engineering literature was introduced to numerical two-dimensional reservoir simulations. Although the Peaceman technique is some empirical recovery approach only, the technique has been developed in Chen and Yue [8], in which a finite element method for some heterogeneous porous media was studied and a rigorous mathematical analysis was presented. Our result may be viewed as a generalization of the excellent work of [8] from two dimensions to three dimensions. However, the generalization is not so straightforward. For instance, the singularity of Green's function in three dimensions is stronger than that in two dimensions, which brings more difficulties to analyze. In the analysis for three-dimensional problems, the corresponding two-dimensional techniques usually need some modifications, too.

Mathematically, our recovered approximation can be viewed as some finite element solution of a regular elliptic problem, in which the singularity is removed. In computation, however, it is more convenient to construct the recovered approximation by using the information of the discrete Green's function G_z^h directly (see Section 3). It is noted that the technique of removing the singularity has been applied to analyze the existence and uniqueness of the nonlinear PBEs (c.f. [7]).

The paper is organized as follows. In the next section, some basic notation is introduced and the $W^{1,p}$ interior estimate for an associated elliptic problem is discussed. The recovery scheme for Green's function approximations is then proposed and analyzed in Section 3. In Section 4, the recovery scheme is applied to some electrostatic potential computations with very satisfactory results. Finally, some concluding remarks are provided.

2. $W^{1,p}$ interior estimate

In this section, we shall introduce some notation and present a $W^{1,p}$ interior estimate for an associated elliptic partial differential equation of the second order, which plays a key role in our analysis of the recover approximation scheme.

Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with Lipschitz boundary $\partial\Omega$. We shall use the standard notation for Sobolev spaces $W^{s,p}(\Omega)$ and their associated norms and seminorms, see, e.g., [1,6]. For $p = 2$, we denote $H^s(\Omega) = W^{s,2}(\Omega)$ and

$H_0^1(\Omega) = \{v \in H^1(\Omega) : v|_{\partial\Omega} = 0\}$, where $v|_{\partial\Omega} = 0$ is in the sense of trace, $\|\cdot\|_{s,\Omega} = \|\cdot\|_{s,2,\Omega}$ and $(\cdot,\cdot)$ is the standard L^2-inner product. In addition, C denotes a generic positive constant which is independent of mesh parameters and may stand for different values at its different occurrences. Define

$$[v]_{2,3,\Omega} = \left(\sup_{x\in\bar{\Omega},0<\rho<+\infty,} \rho^{-3}\int_{\Omega(x,\rho)} |v(y) - v_{\Omega(x,\rho)}|^2 \mathrm{d}y\right)^{1/2}, \tag{2.1}$$

where $\Omega(x,\rho) = B(x,\rho)\cap\Omega$, $B(x,\rho) = \{y \in \mathbb{R}^3 : |y-x| < \rho\}$, and

$$v_D = \frac{1}{|D|}\int_D v(y)\mathrm{d}y$$

is an integral average of the function v over $D \subset \mathbb{R}^3$. Denote $L^c_{2,3}(\Omega)$ as the linear subspace of $L^2(\Omega)$ such that $[v]_{2,3,\Omega} < \infty\, \forall v \in L^c_{2,3}(\Omega)$ and set

$$\|v\|_{L^c_{2,3}(\Omega)} = \left(\|v\|^2_{0,\Omega} + [v]^2_{2,3,\Omega}\right)^{1/2}. \tag{2.2}$$

It is shown in [29] that $(L^c_{2,3}(\Omega), \|\cdot\|_{L^c_{2,3}(\Omega)})$ is a John–Nirenberg space and

$$[v]^2_{2,3,\Omega} \le \inf_{r\in(0,\infty)}\left(\frac{1}{r^3}\|v\|^2_{0,\Omega} + \sup_{x\in\Omega,0<\rho\le r}\rho^{-3}\int_{\Omega(x,\rho)}|v(y) - v_{\Omega(x,\rho)}|^2\mathrm{d}y\right) \quad \forall v \in L^2(\Omega). \tag{2.3}$$

Let Q be a cube in $\mathbb{R}^3$ with the edges parallel to the coordinate axes. For any $v \in L^1(Q)$, define

$$|v|_{*,Q} = \sup_{\tilde{Q}\in\mathbb{Q}}\frac{1}{|\tilde{Q}|}\int_{\tilde{Q}}|v - v_{\tilde{Q}}|\mathrm{d}x,$$

where

$$\mathbb{Q} = \{\tilde{Q} \subset Q : \tilde{Q} \text{ is a cube with edges parallel to the coordinate axes}\}.$$

It is easy to see that $|v|_{*,Q} \le C[v]_{2,3,Q}\forall v \in L^c_{2,3}(Q)$.

The following two lemmas will be used in our analysis concerning the $W^{1,p}$ interior estimate. The first one is nothing but a generalization of (8.2) in [8] to three dimensions and can be verified by the same argument in [8].

Lemma 2.1. *If* $v \in L^c_{2,3}(Q)$, *then*

$$\|v - v_Q\|_{0,p,Q} \le Cp|Q|^{1/p}[v]_{2,3,Q}, \quad p \ge 1. \tag{2.4}$$

The second one is similar to Lemma 8.2 in [8] (c.f. also [29]):

Lemma 2.2. *Suppose* $K_1 \in \mathbb{R}$ *and* $K_1 > 1$. *Let* φ *be a nonnegative increasing function over* $(0, d_0)$. *If the function* $\psi : (0, d_0) \to \mathbb{R}^+$ *satisfies*

$$\psi(\rho) \le K_1\frac{\rho^2}{r^2}\psi(r) + \frac{r^3}{\rho^3}\varphi(r) \tag{2.5}$$

for any $0 < \rho < r < d_0$, *then*

$$\psi(\rho) \le K_1\psi(r) + \frac{K_1^4}{K_1 - 1}\varphi(r), \quad 0 < \rho < r. \tag{2.6}$$

Proof. Following [8], let $l \ge 0$ be the integer such that $1 < K_1^l \le r/\rho \le K_1^{l+1}$. Write (2.5) with ρ replaced by ρK_1^m, r replaced by ρK_1^{m+1} for $m = 0, 1, 2, \ldots, l-1$, we obtain

$$\psi(\rho K_1^m) \le \frac{1}{K_1}\psi(\rho K_1^{m+1}) + K_1^3\varphi(\rho K_1^{m+1}), \quad m = 0, 1, 2, \ldots, l-1.$$

Since φ is an increasing function and $\rho K_1^m < \rho K_1^{m+1} \le r$ $(m = 0, 1, 2, \ldots, l-1)$, we have

$$\psi(\rho K_1^m) \le \frac{1}{K_1}\psi(\rho K_1^{m+1}) + K_1^3\varphi(r), \quad m = 0, 1, 2, \ldots, l-1.$$

Consequently

$$\psi(\rho) \le \left(\frac{1}{K_1}\right)^l \psi(\rho K_1^l) + K_1^3 \varphi(r) \left(1 + \frac{1}{K_1} + \left(\frac{1}{K_1}\right)^2 + \cdots + \left(\frac{1}{K_1}\right)^{l-1}\right). \tag{2.7}$$

It is seen from (2.5) and the nonnegative property of φ that

$$\psi(\rho K_1^l) \le K_1 \psi(r) + K_1^3 \varphi(r). \tag{2.8}$$

Thus inserting (2.8) into (2.7) leads to

$$\begin{aligned}\psi(\rho) &\le \left(\frac{1}{K_1}\right)^l K_1 \psi(r) + K_1^3 \varphi(r) \left(1 + \frac{1}{K_1} + \left(\frac{1}{K_1}\right)^2 + \cdots + \left(\frac{1}{K_1}\right)^{l-1} + \left(\frac{1}{K_1}\right)^l\right) \\ &\le K_1 \psi(r) + \frac{K_1^4}{K_1 - 1} \varphi(r).\end{aligned}$$

This completes the proof. □

Using Lemma 2.2, we are able to generalize the $W^{1,p}$ interior estimate from two dimensions [8] to three dimensions. $W^{1,p}$ interior estimates for elliptic equations are well known in the literature. The importance of the following estimate is the explicit dependence of the bound on p, which plays a key role in our analysis for the recovered approximation.

Proposition 2.1. *Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with Lipschitz boundary. Consider the elliptic equation*

$$Lu := -\sum_{i,j=1}^{3} \frac{\partial}{\partial x_i}\left(a_{ij}(x)\frac{\partial u}{\partial x_j}\right) + b(x)u = \sum_{i=1}^{3} \frac{\partial f_i}{\partial x_i} + f^0 \quad \text{in } \Omega, \tag{2.9}$$

where $a_{ij}(x) \in C^{0,1}(\Omega)$, $b, f_i \in L^\infty(\Omega)$, $f^0 \in L^2(\Omega)$ and there exist $\lambda_1, \lambda_2, \Lambda_1 > 0$ such that $\lambda_1|\xi|^2 \le a_{ij}\xi_i\xi_j \le \lambda_1^{-1}|\xi|^2$, $|b(x)| \le \lambda_2, \forall x \in \bar{\Omega}, \xi \in R^3$, and $|a_{ij}(x) - a_{ij}(y)| \le \Lambda_1|x - y| \forall x, y \in \bar{\Omega}, i, j = 1, 2, 3$. Let $d = \mathrm{diam}(Q)$, $Q \subset \Omega$ be a cube with edges parallel to the coordinate axes such that $\mathrm{dist}(Q, \partial\Omega) \ge C_0 d$ for some constant C_0. Then for any $p > 2$, there exists a constant C depending on λ_1, λ_2 and C_0, such that

$$\|\nabla u\|_{0,p,Q} \le Cp|Q|^{1/p}\left(C_d\|\nabla u\|_{0,\Omega} + d^{-1/2}(\|u\|_{0,\Omega} + \|f^0\|_{0,\Omega}) + \sum_{i=1}^{3}\|f_i\|_{0,\infty,\Omega}\right), \tag{2.10}$$

where $C_d = d^{-3/2} + \Lambda_1 d^{-1/2}$.

Proof. For $x \in Q$, let $r > 0$ such that $B(x, r) \subset \Omega$. It is derived from Lemma 3.2 of [29] that

$$\begin{aligned}\|\nabla u - (\nabla u)_{B(x,\rho)}\|^2_{0,B(x,\rho)} \le C\Bigg(&\frac{\rho^5}{r^5}\|\nabla u - (\nabla u)_{B(x,r)}\|^2_{0,B(x,r)} + \Lambda_1^2 r^2\|\nabla u\|^2_{0,B(x,r)} \\ &+ r^2\|f^0 - bu\|^2_{0,B(x,r)} + \sum_{i=1}^{3}\|f_i - (f_i)_{B(x,r)}\|^2_{0,B(x,r)}\Bigg)\end{aligned}$$

for any $\rho \in (0, r)$. Hence, we may estimate

$$\psi(\rho) = \rho^{-3}\|\nabla u - (\nabla u)_{B(x,\rho)}\|^2_{0,B(x,\rho)} \tag{2.11}$$

as follows

$$\begin{aligned}\psi(\rho) &\le C\left(\frac{\rho^2}{r^2}\psi(r) + \frac{r^3}{\rho^3}\frac{\Lambda_1^2}{r}\|\nabla u\|^2_{0,B(x,r)} + \frac{r^2}{\rho^3}\|f^0 - bu\|^2_{0,B(x,r)} + \rho^{-3}\sum_{i=1}^{3}\|f_i - (f_i)_{B(x,r)}\|^2_{0,B(x,r)}\right) \\ &\le C\left(\frac{\rho^2}{r^2}\psi(r) + \frac{r^3}{\rho^3}\left(\frac{\Lambda_1^2}{r}\|\nabla u\|^2_{0,B(x,r)} + \frac{1}{r}\|f^0 - bu\|^2_{0,B(x,r)} + \sum_{i=1}^{3}[f_i]^2_{2,3,B(x,r)}\right)\right).\end{aligned}$$

Let $d_1 = \mathrm{dist}(Q, \partial\Omega)/2$, then we may choose $r \ge d_1$. Set

$$\varphi(r) = \tilde{C}\left(\Lambda_1^2 d_1^{-1}\|\nabla u\|^2_{0,B(x,r)} + d_1^{-1}\|f^0 - bu\|^2_{0,B(x,r)} + \sum_{i=1}^{3}[f_i]^2_{2,3,B(x,r)}\right)$$

for some constant $\tilde{C} > 0$. Since function $\sum_{i=1}^{3}[f_i]^2_{2,3,B(x,r)}$ increases with r (c.f. [29]), we get that $\varphi(r)$ is an increasing function and

$$\psi(\rho) \le C\frac{\rho^2}{r^2}\psi(r) + \frac{r^3}{\rho^3}\varphi(r), \quad 0 < \rho < r, \tag{2.12}$$

which together with Lemma 2.2 yields

$$\psi(\rho) \le C\left(\psi(r) + \Lambda_1^2 d_1^{-1}\|\nabla u\|^2_{0,B(x,r)} + d_1^{-1}\|f^0 - bu\|^2_{0,B(x,r)} + \sum_{i=1}^{3}[f_i]^2_{2,3,B(x,r)}\right), \quad 0 < \rho < r.$$

Hence, from (2.3) we obtain for $r \ge d_1$ that

$$\begin{aligned}[\nabla u]^2_{2,3,Q} &\le \frac{1}{r^3}\|\nabla u\|^2_{0,\Omega} + \sup_{x\in Q,\ 0<\rho\le r}\psi(\rho)\\ &\le \frac{1}{r^3}\|\nabla u\|^2_{0,\Omega} + C\left(\psi(r) + \Lambda_1^2 d_1^{-1}\|\nabla u\|^2_{0,B(x,r)} + d_1^{-1}\|f^0 - bu\|^2_{0,B(x,r)} + \sum_{i=1}^{3}[f_i]^2_{2,3,B(x,r)}\right).\end{aligned}$$

Let $r = d_1$, then from $\psi(d_1) \le Cd_1^{-3}\|\nabla u\|^2_{0,\Omega}$ we get

$$[\nabla u]^2_{2,3,Q} \le C\left((d_1^{-3} + \Lambda_1^2 d_1^{-1})\|\nabla u\|^2_{0,\Omega} + d_1^{-1}\|f^0 - bu\|^2_{0,\Omega} + \sum_{i=1}^{3}[f_i]^2_{2,3,\Omega}\right).$$

Since $[f_i]_{2,3,\Omega} \le C\|f_i\|_{0,\infty,\Omega}$, we obtain

$$[\nabla u]^2_{2,3,Q} \le C\left((d_1^{-3} + \Lambda_1^2 d_1^{-1})\|\nabla u\|^2_{0,\Omega} + d_1^{-1}\|f^0 - bu\|^2_{0,\Omega} + \sum_{i=1}^{3}\|f_i\|^2_{0,\infty,\Omega}\right).$$

Note that the assumption $\mathrm{dist}(Q, \partial\Omega) \ge C_0 d$ implies $d_1^{-1} \le Cd^{-1}$. Thus combining Lemma 2.1 and the inequality $\|(\nabla u)_Q\|_{0,p,Q} \le C|Q|^{1/p-1/2}\|\nabla u\|_{0,Q}$, we complete the proof. □

3. Finite element recovery scheme

In this section, we study the convergence of the recovery scheme. Let $\Omega \subset \mathbb{R}^3$ be a convex polyhedral domain and $z \in \Omega$. Consider Green's function G_z associated with the singular point z that satisfies

$$\begin{cases}-\mathrm{div}\,(\alpha(x)\nabla G_z) + \beta(x)G_z = \delta_z & \text{in } \Omega,\\ G_z = 0 \quad \text{on } \partial\Omega.\end{cases} \tag{3.1}$$

The coefficients $\alpha(x)$ and $\beta(x)$ are required to have some regularity in our discussion, which is stated as follows.

Assumption 3.1. The coefficients $\alpha \in C^{0,1}(\bar{\Omega})$, $\beta \in L^\infty(\Omega)$ and $\beta(z)/\alpha(z) \ge 0$. Assume there exist constants $\lambda_1, \lambda_2, \Lambda_i(i = 1, 2, 3)$, and $d_z > 0$ such that $\lambda_1 \le \alpha(x) \le \lambda_1^{-1}$, $|\beta(x)| \le \lambda_2\ \forall x \in \bar{\Omega}$,

$$|\alpha(x) - \alpha(y)| \le \Lambda_1|x - y| \quad \forall x, y \in \bar{\Omega}, \tag{3.2}$$

$$|\alpha(x) - \alpha(z)| \le \Lambda_2|x - z|^2, \quad |\beta(x) - \beta(z)| \le \Lambda_3|x - z| \forall x \in \Omega(z, d_z). \tag{3.3}$$

Remark 3.1. For three-dimensional problem (3.1), the assumption $|\alpha(x) - \alpha(z)| \le \Lambda_2|x - z|^2$ is necessary for obtaining some error estimates (see, e.g., (3.13) and (3.14)). It is seen that the condition is satisfied for the PBE, since the coefficient α in the PBE is a piecewise constant. It should be pointed out that the assumption $\alpha \in C^{0,1}(\bar{\Omega})$ is required for obtaining the convergence theoretically. Computationally, however, this assumption is not necessary. Indeed, it is shown by the numerical experiments reported in Section 4 that our recovery scheme may be efficient even for PBEs that are of discontinuous coefficients.

Let $T^h = \{\tau\}$ be a quasi-uniform mesh of Ω with mesh size h (see [6]). Associated with T^h, we define linear finite element spaces by

$$S^h(\Omega) = \{v \in H^1(\Omega) : v|_\tau \in P^1(\tau)\forall\tau \in T^h\}, \qquad S_0^h(\Omega) = S^h(\Omega) \cap H_0^1(\Omega),$$

where $P^1(\tau)$ is the set of linear polynomials over τ.

We introduce the discrete Green's function $G_z^h \in S_0^h(\Omega)$ such that

$$\int_\Omega \left(\alpha(x)\nabla G_z^h \cdot \nabla v_h + \beta(x) G_z^h v_h\right) \mathrm{d}x = v_h(z) \quad \forall v_h \in S_0^h(\Omega). \tag{3.4}$$

It is seen that G_z^h is a finite element solution of G_z and the approximate accuracy of the finite element solution G_z^h is very poor in the vicinity of the singular point z. However, the approximation accuracy will be improved if some reconstruction approach is applied.

Following [8], where $\beta \equiv 0$, let α_z denote $\alpha(z)$ and β_z denote $\beta(z)$. Set $\phi = \exp(-\kappa|x-z|)/(4\pi\alpha_z|x-z|)$, where $\kappa = \sqrt{\beta_z/\alpha_z}$, then ϕ is a solution of the equation

$$\begin{cases} -\mathrm{div}(\alpha_z \nabla\phi) + \beta_z\phi = \delta_z, & x \in \mathbb{R}^3, \\ \phi(\infty) = 0. \end{cases}$$

It is seen that $u \equiv G_z - \phi \in H^1(\Omega)$ satisfying $u = -\phi$ on $\partial\Omega$ and

$$\int_\Omega (\alpha\nabla u \cdot \nabla v + \beta uv)\,\mathrm{d}x = \int_\Omega ((\alpha_z - \alpha)\nabla\phi \cdot \nabla v + (\beta_z - \beta)\phi v)\,\mathrm{d}x \quad \forall v \in H_0^1(\Omega). \tag{3.5}$$

Its finite element approximation u_h satisfies $u_h = -\phi_I$ on $\partial\Omega$ and

$$\int_\Omega (\alpha\nabla u_h \cdot \nabla v_h + \beta u_h v_h)\,\mathrm{d}x = \int_\Omega ((\alpha_z - \alpha)\nabla\phi \cdot \nabla v_h + (\beta_z - \beta)\phi v_h)\,\mathrm{d}x \quad \forall v_h \in S_0^h(\Omega), \tag{3.6}$$

where ϕ_I represents the nodal interpolant of ϕ. Hence we may use $\phi + u_h(z)$ as an approximation to Green's function G_z in the vicinity of the singular point z.

It is significant that $u_h(z)$ can be calculated by using the information of G_z^h directly, which is simpler than obtaining $u_h(z)$ from solving (3.6). In fact, let $\psi_h \in S^h(\Omega)$ be the function whose nodal values are given by

$$\psi_h(x_k) = \begin{cases} -\phi(x_k), & \text{if } x_k \in \partial\Omega, \\ 0, & \text{otherwise}, \end{cases}$$

then $u_h - \psi_h \in S_0^h(\Omega)$ and

$$\begin{aligned} u_h(z) = (u_h - \psi_h)(z) &= \int_\Omega \left(\alpha\nabla G_z^h \cdot \nabla(u_h - \psi_h) + \beta G_z^h (u_h - \psi_h)\right) \mathrm{d}x \\ &= \int_\Omega (\alpha_z - \alpha)\nabla\phi \cdot \nabla G_z^h \mathrm{d}x - \int_\Omega \alpha(x)\nabla G_z^h \cdot \nabla\psi_h \mathrm{d}x + \int_\Omega (\beta_z - \beta)\phi G_z^h \mathrm{d}x - \int_\Omega \beta G_z^h \psi_h \mathrm{d}x, \end{aligned} \tag{3.7}$$

where (3.6) is used.

Consequently, we may construct our recovered approximation as follows

$$\gamma_h(x) = \phi(x) + u_h(z), \tag{3.8}$$

which is used to increase the accuracy of finite element approximation G_z^h near the singularity. Hence, to generate γ_h, it is simpler to calculate $u_h(z)$ by using (3.7) than by solving (3.6).

Next we will analyze this recovered approximation $\gamma_h(x)$ in the vicinity of the singular point z. Denote

$$A_\xi = \{x \in \mathbb{R}^3 : |x - z| = \xi\}, \quad 0 < \xi < \frac{d}{\mathrm{e}^4}, \tag{3.9}$$

where $d = \mathrm{dist}(z, \partial\Omega)$. It is shown by the following theorem that γ_h is a much better approximation than G_z^h over A_ξ.

Theorem 3.1. *If Assumption 3.1 holds, then there exists a constant C independent of h and d but may depend on $\lambda_1, \lambda_2, \Lambda_i$ $(i = 1, 2, 3)$ and the size of the domain such that*

$$\max_{x \in A_\xi} |G_z(x) - \gamma_h(x)| \le C(\tilde{C}_d + d_z^{-1}) \left(\left|\ln\frac{h}{d}\right|^2 + \left|\ln\frac{\xi}{d}\right| \right)(\xi + h), \tag{3.10}$$

where $\tilde{C}_d = \begin{cases} d^{-1/2}, & \text{if } d \ge 1, \\ d^{-7/2}, & \text{if } d < 1, \end{cases}$ d_z and A_ξ are defined respectively in (3.3) and (3.9).

Proof. For any $x \in A_\xi$, from $G_z(x) = u(x) + \phi(x)$ and the construction of $\gamma_h(x)$, we have

$$\begin{aligned} |G_z(x) - \gamma_h(x)| &= |u(x) - u_h(z)| \\ &\le |u(x) - u(z)| + |u(z) - u_h(z)|. \end{aligned} \tag{3.11}$$

Hence, it is sufficient to estimate $|u(x) - u(z)|$ and $|u(z) - u_h(z)|$, respectively.

It is estimated by Proposition 2.1 that

$$\|\nabla u\|_{0,p,B(z,d/4)} \le Cpd^{3/p} \left(C_d\|\nabla u\|_{0,\Omega} + \|(\alpha_z - \alpha)\nabla\phi\|_{0,\infty,\Omega} + d^{-1/2}(\|u\|_{0,\Omega} + \|(\beta_z - \beta)\phi\|_{0,\Omega})\right). \tag{3.12}$$

From (3.5) and Assumption 3.1, we obtain that

$$\|\nabla u\|_{0,\Omega} \le C(\|(\alpha_z - \alpha)\nabla\phi\|_{0,\Omega} + \|(\beta_z - \beta)\phi\|_{0,\Omega} + \|\phi\|_{1,\partial\Omega}) \le Cd^{-2} \tag{3.13}$$

and

$$\|(\alpha_z - \alpha)\nabla\phi\|_{0,\infty,\Omega} \le C \max\{\|(\alpha_z - \alpha)\nabla\phi\|_{0,\infty,B(z,d_z)}, \|(\alpha_z - \alpha)\nabla\phi\|_{0,\infty,\Omega\setminus B(z,d_z)}\} \le Cd_z^{-1}. \tag{3.14}$$

Combining (3.12)–(3.14), we obtain

$$\|\nabla u\|_{0,p,B(z,d/4)} \le Cpd^{3/p}(\tilde{C}_d + d_z^{-1}). \tag{3.15}$$

Using Morrey's embedding theorem [13], we then get

$$\begin{aligned} \max_{x\in A_\xi} |u(x) - u(z)| &\le C(3,p)\xi^{1-3/p}\|\nabla u\|_{0,p,B(z,d/4)} \\ &\le C\xi^{1-3/p}pd^{3/p}(\tilde{C}_d + d_z^{-1}), \end{aligned} \tag{3.16}$$

where the fact that $C(3, p)$ is uniformly bounded for $p > 4$ is used. It is noted from (3.9) that $p = \ln\frac{d}{\xi} > 4$. Thus setting $p = \ln\frac{d}{\xi}$ in (3.16) yields

$$\max_{x\in A_\xi} |u(x) - u(z)| \le C\xi \ln\frac{d}{\xi}(\tilde{C}_d + d_z^{-1}). \tag{3.17}$$

Using the interior L^∞ error estimates of the finite element approximations [24], we arrive at

$$|u(z) - u_h(z)| \le C\left(\left|\ln\frac{d}{h}\right| \inf_{v_h\in S^h(\Omega)} \|u - v_h\|_{0,\infty,B(z,d/4)} + d^{-3/2}\|u - u_h\|_{0,B(z,d/4)}\right). \tag{3.18}$$

To complete the proof, we apply the standard finite element interpolation estimate and (3.15) to obtain

$$\begin{aligned} \inf_{v_h\in S^h(\Omega)} \|u - v_h\|_{0,\infty,B(z,d/4)} &\le Ch^{1-3/p}\|\nabla u\|_{0,p,B(z,d/4)} \\ &\le Ch^{1-3/p}pd^{3/p}(\tilde{C}_d + d_z^{-1}). \end{aligned} \tag{3.19}$$

Taking $p = |\ln\frac{d}{h}|$ in (3.19) we then have

$$\inf_{v_h\in S^h(\Omega)} \|u - v_h\|_{0,\infty,B(z,d/4)} \le Ch\left|\ln\frac{d}{h}\right|(\tilde{C}_d + d_z^{-1}). \tag{3.20}$$

The standard duality argument (c.f. [2]) and (3.13) lead to

$$\begin{aligned} \|u - u_h\|_{0,B(z,d/4)} &\le C(h\|\nabla(u - u_h)\|_{0,\Omega} + h^2\|u - u_h\|_{0,\Omega} + h\|\nabla\phi\|_{0,\partial\Omega}) \\ &\le C(h\|\nabla u\|_{0,\Omega} + h^3\|\nabla u\|_{0,\Omega} + h\|\nabla\phi\|_{0,\partial\Omega}) \\ &\le Chd^{-2}. \end{aligned} \tag{3.21}$$

Thus, combining (3.18), (3.20) and (3.21), we may conclude that

$$|u(z) - u_h(z)| \le Ch\left|\ln\frac{h}{d}\right|^2(\tilde{C}_d + d_z^{-1}). \tag{3.22}$$

Finally, we get (3.10) from (3.11), (3.17) and (3.22). This completes the proof. □

It is derived from Theorem 3.1 that if $|x - z| \le Ch < 1$, then

$$|G_z(x) - \gamma_h(x)| \le Ch \left(\left| \ln \frac{h}{d} \right|^2 + \left| \ln \frac{|x-z|}{d} \right| \right) (\tilde{C}_d + d_z^{-1}). \tag{3.23}$$

Note that the standard error estimate for Green's function approximation is as follows [24],

$$|G_z(x) - G_z^h(x)| \le C \frac{1}{|x-z|}, \quad x \in \Omega \setminus \{z\}. \tag{3.24}$$

Hence γ_h is an highly accurate approximation to G_z in the vicinity of the singular point z.

4. Applications to electrostatic potential computation

In this section, we will apply the recovery scheme to get highly accurate approximations in electrostatic potential computations. Some numerical experiments on uniform finite element meshes are reported for two model problems, which support our theory. One is a potential problem and another is a (linearized) PBE. Our numerical experiments were carried out by SGI Origin 3800 in the State Key Laboratory of Scientific and Engineering Computing, Chinese Academy of Sciences.

The potential problem arises from modeling biomolecular systems with aqueous solvent. It is known that one of the major effects mediated by the aqueous solvent is a screening of the electrostatic interaction. This screening can be formulated by a potential equation [15,25,30]:

$$-\nabla(\epsilon(x)\nabla u(x)) = \sum_{i=1}^{N_m} q_i \delta_{x_i}(x), \tag{4.1}$$

where u is the potential. The dielectric constant

$$\epsilon(x) = \begin{cases} \epsilon_1, & \text{in aqueous solvent region,} \\ \epsilon_2, & \text{in solute molecule region.} \end{cases}$$

The charge distribution in the molecule is represented by a set of point charges $\{q_i \delta_{x_i}\}$ which are located at x_i $(i = 1, \ldots, N_m)$. The potential problem is close to the PBE and can be viewed as a simplified model for electrostatics.

Example 4.1 (*[30]*). Consider the following potential problem

$$\begin{cases} -\nabla(\epsilon(x)\nabla u(x)) = q_0 \delta_0(x) & \text{in } \Omega, \\ u = g \quad \text{on } \partial\Omega, \end{cases} \tag{4.2}$$

where $\delta_0(x) = \delta_{(0,0,0)}(x)$. The entire solution domain $\Omega = (-2, 2)^3$, the molecular domain $\{x \in \mathbb{R}^3 : |x| \le 1\}$, and the coefficient

$$\epsilon(x) = \begin{cases} \epsilon_1 = 1, & |x| < 1, \\ \epsilon_2 = 80, & |x| > 1. \end{cases}$$

The molecule has a charge $q_0 = 1$ that is located at the origin $(0, 0, 0)$ and $g(x)$ is given by the exact solution

$$u(x) = \begin{cases} \dfrac{1}{4\pi\epsilon_1|x|} + \dfrac{1}{4\pi}\left(\dfrac{1}{\epsilon_2} - \dfrac{1}{\epsilon_1}\right), & |x| \le 1, \\ \dfrac{1}{4\pi\epsilon_2|x|}, & |x| < 1. \end{cases}$$

The approximate errors and convergence rates of the two approximations at $x_0 = (1/256, 0, 0)$ (a point in the vicinity of singular point $(0, 0, 0)$) are provided in Table 1. Here $|(u - u_h)(x_0)|$ represents the absolute error between u and its finite element approximation u_h on x_0. Denote by γ_h the recovered approximation to u. It is shown by the last column of Table 1 that the convergence rate of γ_h approximates to 1.0. This implies the error $|(u - \gamma_h)(x_0)| = O(h)$, which is much better than that of the finite element solution u_h and agrees with our theory (see (3.23)), though the coefficient of (4.2) does not satisfy Assumption 3.1. More precisely, the ratio of $|(u - u_h)(x_0)|$ and $|(u - \gamma_h)(x_0)|$ is about 1:6000 if about 270,000 degrees of freedom of the discretizations are used.

Our second experiment is to solve a linearized PBE. Consider a spherical molecule with charge q located at the origin in a solvent containing mobile univalent ions (see Fig. 1). The radius of the molecule is denoted by R. The entire region Ω can be divided into three regions. The molecule in which we wish to determine the electrostatic potential is located at $\Omega_1 = \{x \in \mathbb{R}^3 : |x| < R\}$, region $\Omega_2 = \{x \in \mathbb{R}^3 : R < |x| < a\}$ is an ion-exclusion layer around the molecule in which

Table 1
Error and convergence rate for the recovery scheme (Example 4.1)

h	DOFs	$\|(u-u_h)(x_0)\|$	Rate	$\|(u-\gamma_h)(x_0)\|$	Rate
1	125	20.2832	\	0.04835	\
1/2	729	19.8936	0.02799	0.01482	1.7056
1/4	4913	19.3837	0.03746	0.009284	0.6751
1/8	35 937	18.3973	0.07535	0.005277	0.8149
1/16	274 625	16.4974	0.1573	0.002803	0.9128

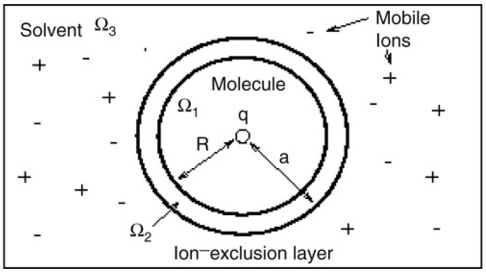

Fig. 1. Spherical molecule (see [15]).

no mobile charges of the solvent are present, the ionic solvent lies in region Ω_3 and $\bar{\Omega}_1 \cup \bar{\Omega}_2 \cup \bar{\Omega}_3 = \bar{\Omega}$. The electrostatic potential of the molecule in the solvent in $\Omega = \mathbb{R}^3$ can be formulated as follows [12,14,15,19,25,31]

$$\begin{cases} -\nabla(\epsilon(x)\nabla u(x)) + \bar{\kappa}^2(x)u(x) = 4\pi q\delta_0(x) & \text{in } \mathbb{R}^3, \\ u(\infty) = 0, \end{cases} \tag{4.3}$$

where

$$\epsilon(x) = \begin{cases} \epsilon_1, & x \in \Omega_1, \\ \epsilon_2, & x \in \Omega_2, \\ \epsilon_3, & x \in \Omega_3, \end{cases} \quad \bar{\kappa}(x) = \begin{cases} 0, & x \in \Omega_1 \text{ or } \Omega_2, \\ \sqrt{\epsilon_3}\kappa, & x \in \Omega_3. \end{cases} \tag{4.4}$$

For this special case, the analytical solution can be explicitly expressed as follows:

$$u(r) = \begin{cases} \dfrac{q}{\epsilon_3 a(1+\kappa a)} + \dfrac{q}{R}\left(\dfrac{1}{\epsilon_2} - \dfrac{1}{\epsilon_1}\right) - \dfrac{q}{\epsilon_2 a} + \dfrac{q}{\epsilon_1}\dfrac{1}{r}, & 0 \le r \le R, \\ \dfrac{q}{\epsilon_3 a(1+\kappa a)} - \dfrac{q}{\epsilon_2 a} + \dfrac{q}{\epsilon_2}\dfrac{1}{r}, & R < r \le a, \\ \dfrac{q\exp(\kappa a)}{\epsilon_3(1+\kappa a)}\dfrac{\exp(-\kappa r)}{r}, & r > a, \end{cases} \tag{4.5}$$

where $r = |x|$.

Example 4.2 (*c.f.* [15,16]). Suppose $R = a$ and $\epsilon_1 = \epsilon_2$ in (4.3) and (4.4). Consider the entire domain $\Omega = (-2a, 2a)^3$ and the molecular area $\Omega_1 = \{x \in \mathbb{R}^3 : |x| < a\}$, $a = 0.25$ Å. Then the simplified problem is as follows:

$$\begin{cases} -\nabla(\epsilon(x)\nabla u(x)) + \bar{\kappa}^2(x)u(x) = 4\pi q\delta_0(x) & \text{in } \Omega, \\ u(x) = g(x) & \text{on } \partial\Omega. \end{cases}$$

The discontinuous coefficients are

$$\epsilon(x) = \begin{cases} \epsilon_1 = 1, & 0 \le |x| < a, \\ \epsilon_3 = 80, & |x| > a, \end{cases} \quad \bar{\kappa}^2(x) = \begin{cases} 0, & 0 \le |x| < a, \\ \kappa^2\epsilon_3, & |x| > a, \end{cases}$$

where the Debye–Hückel parameter $\kappa = 0.102998197$. The boundary condition is given by the exact solution

$$u(x) = \begin{cases} \dfrac{q}{\epsilon_3(1+\kappa a)} - \dfrac{q}{\epsilon_1 a} + \dfrac{q}{\epsilon_1|x|}, & 0 \le |x| \le a, \\ \dfrac{q\exp(\kappa a)}{\epsilon_3(1+\kappa a)}\dfrac{\exp(-\kappa|x|)}{|x|}, & |x| > a. \end{cases}$$

The numerical results for Example 4.2 are reported in Table 2, where $x_0 = (4.88 \times 10^{-4}, 0, 0)$. Different from problem (4.2), the exact solution u of this problem is very small, which leads to the smallness of the absolute errors displayed in Table 2. For this PBE, the convergence rate of γ_h also approximates to 1.0, which implies that the recovery scheme is very efficient and supports our theory.

Table 2
Error and convergence rate for the recovery scheme (Example 4.2)

h	DOFs	$\|(u-u_h)(x_0)\|$	Rate	$\|(u-\gamma_h)(x_0)\|$	Rate
1/8	729	0.9721e−6	\	0.3479e−9	\
1/16	4913	0.9597e−6	0.0185	0.2142e−9	0.6997
1/32	35 937	0.9355e−6	0.0368	0.1177e−9	0.8638
1/64	274 625	0.8881e−6	0.0750	0.05822e−9	1.0155
1/128	2146 689	0.7965e−6	0.1570	0.02920e−9	0.9955

5. Concluding remarks

In this paper, we have constructed and analyzed a finite element recovery scheme which can produce highly accurate approximations to Green's functions. It is proved by both theory and numerical experiments that this scheme is very efficient. In particular, the recovery scheme has been successfully applied to some electrostatic potential computations, which is based on a linearized PBE. The linearized PBE is a simple version of the following nonlinear PBE by using an approximation $(\sinh(x) \sim x)$

$$\begin{cases} -\nabla(\epsilon(x)\nabla\phi(x)) + \bar{\kappa}^2(x)\left(\dfrac{k_BT}{e_c}\right)\sinh\left(\dfrac{e_c\phi(x)}{k_BT}\right) = 4\pi e_c \displaystyle\sum_{i=1}^{N_m} z_i\delta_{x_i}(x) \quad \text{in } \mathbb{R}^3, \\ \phi(\infty) = 0, \end{cases} \tag{5.1}$$

where constants k_B and T represent Boltzmann's constant and absolute temperature, respectively, and the other parameters are the same as that in (1.1). This model has been extensively used to compute the electrostatic potential of biomolecules (see, e.g., [3,12,15,17,22,26] and references cited therein). It is noted that in most biologically relevant cases ϕ is not very small. Notwithstanding this fact, the solution obtained from the linearized PBE is close to the solution obtained from the nonlinear PBE, even if the linearization condition does not hold (see, e.g., [12,14,15,19,25,31]). Moreover, although the nonlinearity increases the difficulty of numerical computation, the main computational difficulty comes from the point singularity. In our forthcoming work, we will study and apply the recovery scheme to solve nonlinear PBEs.

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